CASC Center for Applied
Scientific Computing

University of California
**Lawrence Livermore
National Laboratory**

ISCR
Annual Report

FY1998

ISCR

Institute for Scientific Computing Research

The University Relations Program (URP) encourages collaborative research between Lawrence Livermore National Laboratory (LLNL) and the University of California campuses. The Institute for Scientific Computing Research (ISCR) actively participates in such collaborative research, and this report details the Fiscal Year 1998 projects jointly served by URP and ISCR. For a full discussion of all URP projects in FY 1998, please request a copy of the URP FY 1998 Annual Report by contacting

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UCRL-LR-133866-98

ISCR Fiscal Year 1998 Report

Advances in scientific computing research have never been more vital to the core missions of Lawrence Livermore National Laboratory than they are today. These advances are evolving so rapidly, and over such a broad front of computational science, that to remain on the leading edge, the Laboratory must collaborate with many academic centers of excellence. In FY 1998, ISCR dramatically expanded its interactions with academia through collaborations, visiting faculty, guests and a seminar series. The pages of this annual report summarize the activities of the 63 faculty members and 34 students who participated in ISCR collaborative activities during FY 1998.

The 1998 ISCR call for proposals issued by the University Collaborative Research Program (UCRP) resulted in eight awards made by the University of California Office of the President to research teams at UC San Diego, UC Davis, UC Los Angeles, and UC Berkeley. These projects are noted below.
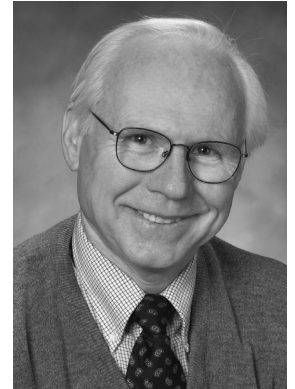
John M. Fitzgerald
Acting Director, ISCR

Software Infrastructure for Multi-Tier Implementation of Structured Adaptive Mesh Hierarchies

Professor Scott Baden, UCSD
LLNL collaborator, Jonathan May (CASC)

A Computational Investigation of Finite-Strain Plasticity Models for Crystalline Solids

Professor Panayiotis Papadopoulos, UCB
LLNL collaborator, Daniel J. Nikkel Jr. (ME)

Massively Parallel Computation Applied to Finite Element Analysis

Professor Tony Keaveny, UCB
LLNL collaborator, Karin Hollerbach (CASC)

Computational Fluid Dynamic Studies of Arterial Flow Disturbances Induced by Intravascular Stents

Professor Abdul Barakat, UCD
LLNL collaborator, Patrick Fitch (BBRP)

Parallel Multigrid Methods on Unstructured Grids for Scientific Computing

Professor Tony Chan, UCLA
LLNL collaborator, Robert Falgout (CASC)

Parallel Particle-in-Code Modeling of Semiclassical Quantum Models

Professor Viktor Decyk, UCLA
Professor John M. Dawson, UCLA
LLNL collaborator, Dennis Hewett (CASC)

Development of a Three-Dimensional Relativistic Particle-In-Cell Code for Studying the Production of Useful Electron Bunches Using Ultra-Intense Laser Pulses

Prof Warren B. Mori, UCLA
LLNL collaborator, Scott Wilks (X-Division)

Methods of Simulation for Localized Multiply-Scaled Condensed Materials

Professor John Weare, UCSD
LLNL collaborator, Scott Kohn (CASC)

ISCR is now part of the Laboratory's Center for Applied Scientific Computing (CASC). Many CASC scientists participate actively in ISCR–University collaborations, as noted. The eight collaborations shown represent innovative research efforts supported by ISCR in FY 1998. Abstracts discussing each of these collaborations begin on page 79.

The Accelerated Strategic Computing Initiative (ASCI) established Academic Strategic Alliances Program (ASAP) centers located at: Stanford University; California Institute of Technology; University of Chicago; University of Utah, Salt Lake; and University of Illinois, Urbana-Champaign.

The ASCI Alliances strategy was established to enhance overall ASCI goals by establishing technical interactions between the Department of Energy, Defense Programs laboratories (Lawrence Livermore, Los Alamos, and Sandia National Laboratories), and leading-edge research-and-development universities in the United States.

ISCR has partnered with the LLNL ASCI Program Office to facilitate these collaborations. In FY 1998, ISCR hosted ASCI Alliances student guests who visited LLNL for collaborations during the summer months.

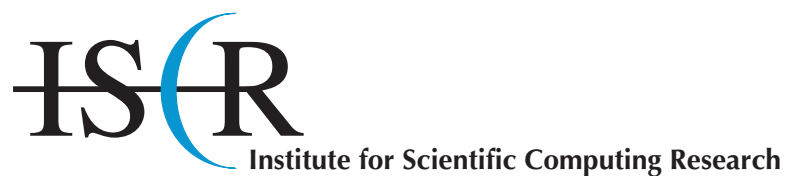We hope that you enjoy this report on ISCR's many activities throughout FY 1998. For further information about the Institute, please contact me at your convenience.

John Fitzgerald
Acting Director

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Contents

ISCR Institute for Scientific Computing Research

FY 1998 Seminar Series
(in reverse chronological order)

Michael Pernice, University of Utah	September 29, 1998
Dean Dauger, University of California, Los Angeles	September 28, 1998
Malvin H. Kalos, Cornell University	September 23, 1998
Steven Lumetta, University of Illinois, Urbana-Champaign	September 17, 1998
Leonid Oliker, NASA Ames Research Center	September 11, 1998
Roger L. Haskin, IBM Almaden Research Center	September 3, 1998
Jonathan Dursi, University of Chicago	August 31, 1998
Yuan-Nan Young, University of Chicago	August 31, 1998
Abraham Szoke, Lawrence Livermore National Laboratory	August 25, 1998
Timothy Barth, Numerical Aerospace Simulation, NASA	August 24, 1998
Dave Beazley, University of Chicago	August 21, 1998
Steve Parker, University of Utah	August 19, 1998
Louiqa Raschid, University of Maryland	August 15, 1998
Michael Franklin, University of Maryland	August 15, 1998
Harland Glaz, University of Maryland	August 12, 1998
Karen L. Karavanic, University of Wisconsin, Madison	August 7, 1998
Howard Elman, University of Maryland	July 31, 1998
George Bebis, University of Nevada, Reno	July 22, 1998
Chris Brislawn, Los Alamos National Laboratory	July 17, 1998
Andrew Grimshaw, University of Virginia	July 10, 1998
Bernd Hamann, University of California, Davis	July 1, 1998
Raytcho Lazarov, Texas A & M University	June 29, 1998
Ulrich Ruede, Universitaet Augsburg	June 25, 1998
Dirk Grunwald, University of Colorado, Boulder	June 19, 1998
Roland Freund, Bell Labs	June 18, 1998
Ian Foster, Argonne National Laboratory	June 16, 1998
Laura Myers Haas, IBM Almaden	June 12, 1998
Dimitri Mavriplis, ICASE, NASA Langley	June 11, 1998
David Keyes, Old Dominion University	May 29, 1998
Hongyhan Zha, Pennsylvania State University	May 22, 1998
Jack Dongarra, University of Tennessee	May 19, 1998
Chandrajit L. Bajaj, University of Texas at Austin	May 1, 1998
Dean H. Judson, University of Nevada	April 28, 1998
Paul Dubois, Lawrence Livermore National Laboratory	April 20, 1998
Raghu Machiraju, Mississippi State University	April 17, 1998

Center for Applied Scientific Computing

Nabil Adam, Rutgers University   April 17, 1998
    and Igg Adiwijaya, Rutgers University
Peter Schroeder, California Institute of Technology   April 14, 1998
Kenneth I. Joy, University of California, Davis   April 10, 1998
Malvin H. Kalos, Cornell University   March 30, 1998
Ann Hollister, Louisiana State Univ. Medical Center   March 27, 1998
Louise Focht, Avanta Orthopedics, Inc.   March 27, 1998
Jinchao Xu, Penn State University   March 20, 1998
Jesse Barlow, Penn State University   March 19, 1998
John Feo, Tera Computers   March 9, 1998
Tamara G. Kolda, Oak Ridge National Laboratory   February 26, 1998
John Bell, Lawrence Berkeley National Laboratory   February 24, 1998
Sam Uselton, Numerical Aerospace Simulation, NASA   February 20, 1998
Paul Woodward, University of Minnesota   February 20, 1998
Kathy Holian, Los Alamos National Laboratory   February 11, 1998
Dan Quinlan, Los Alamos National Laboratory   February 6, 1998
Michael Holst, University of California, Irvine   January 16, 1998
David Keyes, Old Dominion University   December 19, 1997
David H. Bailey, NASA Ames Research Center   December 16, 1997
James Browne, University of Texas at Austin   December 12, 1997
Thomas F. Russell, University of Colorado, Denver   December 9, 1997
Randy Bank, University of California San Diego   November 11, 1997
Sing-Lok (Justin) Wan, Univ. of California, Los Angeles   November 10, 1997

Visitors, Guests, Consultants, and Researchers

Sabbatical Visitor

Raytcho Lazarov, Texas A&M University

Participating Guests

Marsha Berger, New York University
George Byrne, Illinois Institute of Technology
David Dean, University of Colorado
Harry Dwyer, University of California, Davis
Alejandro Garcia, San Jose State University
Bernd Hamann, University of California, Davis
Stanley Johnson, Lehigh University
Joel Kaiser, University of California, Davis
Martin Lades, Genetrace
David Larson, Bay Area Research Corporation
Gerry Elbridge Puckett, University of California, Davis
Yousef Saad, University of Minnesota
Paul Saylor, University of Illinois, Urbana-Champaign
Jeffrey Scoggs, North Carolina State University
Kenneth Trauner, University of California, Davis Medical School
Daniel Wake, TMA, Inc.

Consultants

Berni Alder, University of California Professor Emeritus
Randolph Bank, University of California San Diego
Anne Greenbaum, University of Washington
Thomas Manteuffel, University of Colorado
Stephen McCormick, University of Colorado
Linda Petzold, University of California, Santa Barbara
Steve Schaffer, New Mexico Tech
Homer Walker, Worcester Polytechnic Institute

Visitors

Marian Brezina, University of Colorado
David Brown, Los Alamos National Laboratory
Larry Carter, University of California, San Diego
Angela Cheer, University of California, Davis
Al Davis, University of Utah
Harry Dwyer, University of California, Davis
James Demmel, University of California, Berkeley
Oliver Duschka, Socratix System
Raymond Scott Fellers II, University of California, Berkeley
Ernesto Gomez, University of Chicago
Charles Hansen, University of Utah
Thomas Henderson, University of Utah
Michael Allen Heroux, Sandia National Laboratories Albuquerque
Chris Johnson, University of Utah
Joel Kaiser, University of California, Davis
Thomas Ivan Milac, University of Washington
Lloyd Minick, Socratix System
Mark Alan Musan, Stanford University and Socratix System
Esmond Gee-Ying Ng, Oak Ridge National Laboratory
Julia Elizabeth Rice, IBM Almaden
Jennifer M. Schopf, University of California, San Diego
Andrew P. Strelzoff, University of California, Santa Barbara
Wei-Pai Tang, University of Waterloo
Kathleen Thompson, Socratix System
Angus Taylor, University of California, Berkeley
Michael Tocci, Worcester Polytechnic Institute

Visitors, Guests, Consultants, and Researchers (cont.)

Subcontracts, ASCI Level 3

Bruce Boghosian, Boston University
David Keyes, Old Dominion University
John Ruge, Front Range Scientific Computation, Inc.

University Collaborative Research Program Proposals

Scott Baden, University of California, San Diego
Abdul Barakat, University of California, Davis
Tony Chan, University of California, Los Angeles
Viktor Decyk and John Dawson, University of California, Los Angeles
Tony Keaveny, University of California, Berkeley
Warren Mori, University of California, Los Angeles
Panayiotis Papadopoulos, University of California, Berkeley
John Weare, University of California, San Diego

LDRD Projects

Karin Hollerbach, LLNL Center for Applied Scientific Computing
Peter Brown, LLNL Center for Applied Scientific Computing

Postdoctoral Researchers

Raymond S. Fellers II
Madhaven Ganesh
Brian J. Miller
Thomas F. Rutaganira

Students and Faculty

Department of Applied Science Faculty

Nelson L. Max
Garry H. Rodrique

Department of Applied Science Students

Paul E. Covello
David S. Miller
Johnathan E. Rochez
Jay Feltus Thomas

Visiting Students and Faculty

Mark Adams, University of California, Berkeley
Igg Adiwijaya, Rutgers University
Travis Austin, University of Colorado, Boulder
Lora Ballinger, University of Utah
George Bebis, University of Nevada, Reno
Martin Bertram, University of California, Davis
Kathleen Bonnell, California State University, Dominguez Hills
Dan Bullok, University of Illinois
Tim Chartier, University of Colorado, Boulder
Jonathan Dursi, University of Chicago
Chris Higginson, University of Colorado, Boulder
Rithea Hong, Texas A&M University
Rachel Karchin, Stanford University
Falko Kuester, University of California, Davis
Jonathan Pearlman, University of California, Berkeley
Lyn Reid, University of Washington
Natasha Sager, Las Positas Junior College
Michael Wittman, University of California, Davis
Yuan-Nan Young, University of Chicago

Students and Faculty (cont.)

National Physical Science Consortium (NPSC)

Lora Ballinger, University of Utah
Rachel Karchin, Stanford University
Imelda Kirby, University of Arizona
Megan Thomas, University of California, Davis